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TITLE: REGIONAL AIR QUALITY IN THE FOUR CORNERS STUDY REGION: MODELING APPROACH

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REGIONAL AIR QUALITY IN THE FOUR CORNERS STUDY REGION: MODELING APPROACH

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1. INTRODUCTION

The modeling methodology used in the regional air quality analysis for the Four Corners Study Region and some sample results are discussed in this paper. The boundaries of the study region are shown in Figure 1. The Four Corners Study was one of five regional studies conducted for the National Commission on Air Quality. A more detailed discussion of the regional air quality analysis is presented elsewhere (Mochumson, 1981). A description of the alternative scenarios and regulatory policies that were evaluated is presented in a report by Roach et al. (1981).

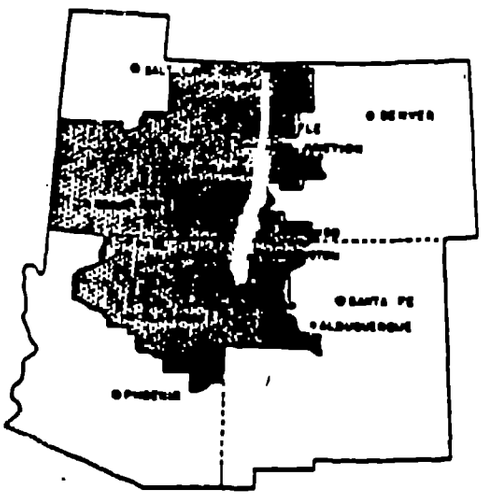

Figure 1. The Four Corners Study Region

A two-dimensional Eulerian air pollutant transport model was used to estimate the concentration and deposition of sulfur dioxide (SO_2), particulate sulfates (SO_4), and primary fine particulates (FPM) on an annual average basis. The model accounts for the atmospheric processes of advective transport, transformation, dispersion and wet and dry deposition. The outputs from this model were also used as inputs to regional atmospheric visibility and mass budget calculations. The concentrations and depositions were estimated for 1° by 1° grid cells that extend vertically to the top of the mixing layer and that cover the Four Corners States (Figure 2). The study region emissions were apportioned to the grid array elements according to emission source location. One major advantage of the transport model employed is that its solution involves the calculation of transfer coefficients which relate air pollution emissions directly to ambient concentrations and dry and wet deposition.

A simplified version of the model was shown to give estimates of ambient sulfate concentrations which compared well with observations (Mochumson, 1978). When the model was used with methods for calculating the contribution of SO_4 to regional atmospheric visibility reduction (Mochumson, 1981), the model's estimates were consistent with estimates from historical relationships between sulfur oxide emissions and regional visibility reported by Mariana and Trijonis (1979).

2. METHODOLOGY

The model is derived from mass balance equations for primary and secondary pollutants for a system of cells in a two-dimensional array (Mochumson, 1978). The secondary pollutant is formed through the chemical conversion of the primary pollutant. The model is analogous to a two-dimensional estuarine water quality model (Thomann, 1972). The model accounts for the following atmospheric processes.

- The transformation of the primary to the secondary pollutant.
- The wet and dry deposition of the primary and secondary pollutants.
- The advective transport between cells.
- Vertical mixing up to the top of the mixing layer.

The model is solved for the steady-state case. The model can be used to make long term average (weeks to years) concentration and deposition estimates. The following assumptions were made.

- There is no interchange at the top of the mixing layer.
- There is complete mixing within the boundaries of each cell.
- Horizontal dispersion is unimportant relative to advection.
- The transformation and/or removal terms of the mass balance equations are first order in primary and/or secondary pollutant concentrations.

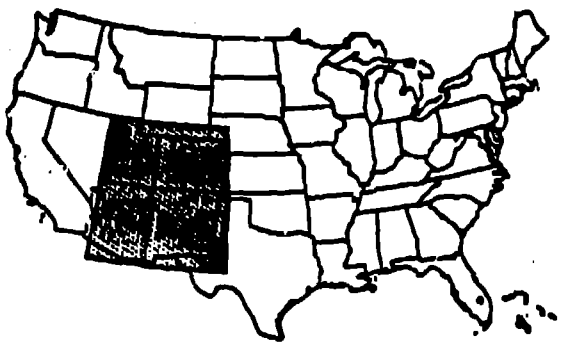

Figure 2. Boundaries for the regional air quality modeling.

- The wet removal terms of the mass balance equations are first order in the rate of precipitation.

The input and output variables and the parameters of the model are presented in Table 1.

2.1 Model Equations

The model is derived from the following mass balance equations for the primary and the secondary pollutants.

Mass Balance Equation for the Primary Pollutant:

$$\frac{dc_{1i}}{dt} V_i = E_{1i} + F_{1Ii} - F_{1Oi} -$$

Accumulation; Emissions; Advective Transport In; Advective Transport Out

$$k_{ti} c_{1i} V_i - k_{r1i} c_{1i} V_i + F_{1Ibi} - F_{1Obi} \quad (1)$$

Transformation; Removal; Advective Transport In At The Boundary; Advective Transport Out At The Boundary

Mass Balance Equation for the Secondary Pollutant:

$$\frac{dc_{2i}}{dt} V_i = E_{2i} + F_{2Ii} - F_{2Oi} + \delta k_{ti} c_{1i} V_i -$$

Accumulation; Emissions; Advective Transport In; Advective Transport Out; Transformation

$$k_{r2i} c_{2i} V_i + F_{2Ibi} - F_{2Obi} \quad (2)$$

Removal; Advective Transport In At The Boundary; Advective Transport Out At The Boundary

where

$$F_{kIi} = \sum_{j \neq i} c_{kji} U_{ji} \quad (3)$$

$$F_{kOi} = \sum_{j \neq i} c_{kij} U_{ij} \quad (4)$$

$$F_{kIbi} = \sum_{b} c_{kbi} U_{bi} \quad (5)$$

$$F_{kObi} = \sum_{b} c_{kib} U_{ib} \quad (6)$$

$$c_{kji} = a_{kji} c_{kj} + (1 - a_{kji}) c_{ki} \quad (7)$$

$$c_{kij} = a_{kij} c_{ki} + (1 - a_{kij}) c_{kj} \quad (8)$$

$$c_{kbi} = a_{kbi} c_{kbi} + (1 - a_{kbi}) c_{ki} \quad (9)$$

$$c_{kib} = a_{kib} c_{ki} + (1 - a_{kib}) c_{kbi} \quad (10)$$

TABLE 1

INPUT-OUTPUT VARIABLES AND MODEL PARAMETERS

Input Variables[a]

- Primary and secondary pollutant emission rates
- Mixing layer height
- Two-dimensional air flow within the mixing layer (frequency of direction and speed normal to the grid cell faces)
- Precipitation
- Cell dimensions

Output Variables[a,c]

- Concentration
- Deposition

Parameters[a,c]

- Conversion rate for the primary pollutant
- Dry deposition velocities[c]
- Wet deposition rate constants[c]

[a]By grid cell and averaging period.
[b]They are lumped parameters representing averages values over space (grid cell) and time (averaging time).
[c]For primary and secondary pollutants

$$U_{ji} = w_{ji} H u_{ji} \quad (11)$$

$$U_{ij} = w_{ij} H u_{ij} \quad (12)$$

$$U_{bi} = w_{bi} H u_{ij} \quad (13)$$

$$U_{ib} = w_{ib} H u_{ib} \quad (14)$$

$$w_{ji} = w_{ij} \quad (15)$$

$$w_{ib} = w_{bi} \quad (16)$$

$$V_i = A_i H \quad (17)$$

$$k_{rki} = (V_{dki}/H) + k_{wdki} P_i \quad (18)$$

$$\delta = M_2/M_1 \quad (19)$$

For all cells within the grid array, Eqs. (1) and (2) under the assumption of steady-state

comprise a system of linear equations that can be expressed as the following matrix equations:

$$A_1 C_1 = Q_1 + B_1 \quad (20)$$

$$A_2 C_2 = Q_2 + C_1 + B_2 \quad , \quad (21)$$

where

$$A_k = \begin{bmatrix} a_{k11} & \cdots & a_{k1n} \\ \cdot & & \cdot \\ a_{kn1} & \cdots & a_{knn} \end{bmatrix} \quad (22) \qquad C_k = \begin{bmatrix} c_{k1} \\ \cdot \\ c_{kn} \end{bmatrix} \quad (23)$$

$$Q_k = \begin{bmatrix} Q_{k1} \\ \cdot \\ \cdot \\ \cdot \\ Q_{kn} \end{bmatrix} \quad (24) \qquad B_k = \begin{bmatrix} b_{k1} \\ \cdot \\ \cdot \\ \cdot \\ b_{kn} \end{bmatrix} \quad (25)$$

$$a_{11i} = -\sum_{j \neq i} [(1 - \alpha_{1ji})U_{ji} - \alpha_{1ij} U_{ij}] - \sum_b [(1 - \alpha_{1bi})U_{bi} - \alpha_{11b}U_{1b}] + (k_{ti} + k_{r1i})V_i \quad . \quad (26)$$

$$a_{11j} = -\alpha_{1ji}U_{ji} + (1 - \alpha_{11j})U_{ij} \quad (27)$$

$$b_{1i} = \sum_b \alpha_{1bi}[\alpha_{1bi}U_{bi} + (1 - \alpha_{11b})U_{1b}] \quad (28)$$

$$Q_{1i} = E_{1i} \quad (29)$$

$$a_{21i} = (-\sum_{j \neq i} [(1 - \alpha_{2ji})U_{ji} - \alpha_{21j}U_{ij}] - \sum_b [(1 - \alpha_{2bi})U_{bi} - \alpha_{21b}U_{1b}] + k_{r2i} V_i)/(\delta k_{ti}V_i) \quad (30)$$

$$a_{21j} = [-\alpha_{2ji}U_{ji} + (1 - \alpha_{21j})U_{ij}]/(\delta k_t V_i) \quad (31)$$

$$b_{2i} = (\sum_b \alpha_{2bi}[\alpha_{2bi}U_{bi} + (1 - \alpha_{21b})U_{1b}])/(\delta k_t V_i) \quad (32)$$

$$Q_{2i} = E_{2i}/(\delta k_t V_i) \quad (33)$$

The elements of the matrix inverse of A_1 represent transfer coefficients between primary emissions, E_{1i}, or boundary elements, b_{1i}, and primary concentrations, c_{1i}. The elements of the matrix inverse of A_2 represent transfer coefficients between primary concentrations, c_{1i}, secondary factorized emissions, Q_{2i}, or factorized boundary elements, b_{2i}, and secondary concentrations, c_{2i}. The transfer coefficients need to be calculated only once for a given time period and set of model parameters and can be used repeatedly for the analysis of alternative scenario policies with different emission source configurations. FPM can be modeled by employing Eq. (30) and setting $k_t = 0$.

2.2 Model Parameters and Meteorological Variables

The model parameters for SO_2, SO_4, and FPM used in the study and presented in Tables 2 and 3 are typical of values found in the air pollution literature (Nochumson, 1978). A relatively low transformation rate of 0.5% per hour was used to represent the transformation of SO_2 to SO_4 in the relatively clean non-reactive southwestern atmosphere. The wet deposition rate parameter was based on long-term average sulfur oxide concentration and wet deposition measurements in the northeastern US (Nochumson, 1978). The precipitation rates were based on data reported by the National Weather Service (1967-1971). The mixing height was based on data reported by Holzworth (1972). The two-dimensional wind field was based on upper 850 mb wind data prepared by Crutcher (1961).

TABLE 2

SPECIES-INDEPENDENT MODEL PARAMETERS

Parameter	Value	Units
α	0.9	-
δ	1.5	-
H	1405.0	m

TABLE 3

SPECIES-DEPENDENT MODEL PARAMETERS

Parameter	Sulfur Dioxide	Volve Particulate Sulfates	Primary Fine Particulates	Units
k_t	1.4×10^{-6}	---	---	s^{-1}
V_d	0.01	0.002	0.002	m/s
k_{wd}	1.4×10^{-7}	1.4×10^{-7}	1.4×10^{-7}	s^{-1}/(in/yr)

3. RESULTS

Some sample results from the regional air quality analysis completed for the Four Corners Study are presented in this section. A more detailed discussion of the results is presented elsewhere (Nochumson, 1981). Isopleths of annual average sulfate concentrations calculated for the 1980 baseline year from the sulfur oxide emission sources located within the study region are shown in Figure 3. Secondary pollutants formed by the chemical conversion of primary pollutants such as SO_4, which is formed by the atmospheric oxidation of SO_2, have much more gradual spatial gradients in concentration than primary pollutants. Secondary pollutants formed by chemical conversion or condensation of gases such as SO_4 are fine particulate matter and are found primarily in the accumulation mode size range, 0.2-2 um in diameter. Particules in this size range have a high residence time in the atmosphere because they are slow to be removed by dry deposition

processes. They are believed to be slow in being transported by Brownian diffusion across the laminar boundary layer at the earth's surface. For this reason, they can be transported over long distances (hundreds to thousands of kilometers) before being completely removed from the atmosphere.

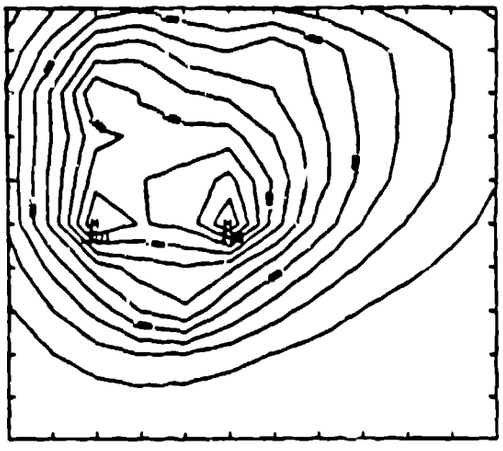

Figure 3. Particulate sulfate concentrations isopleths for the 1980 baseline year under current regulations (ug/m^3).

The fate of SO_2, SO_4, and FPM was examined through regional budget calculations based on the results from the regional air quality modeling. We estimated the amounts of SO_2, SO_4, and FPM emitted in the study region, deposited by dry and wet removal processes, and advected out of a control volume over the Four Corners States (see Table 4). The control volume extends to the top of the mixing layer and its perimeter is shown in Fig. 2. The budgets were estimated for the 1980 baseline year and for three scenario-years, the mid-scenario in 1987 and 1995 and the hi h scenario in 1995. Approximately equal amounts of the SO_4 and FPM were estimated to be removed from the atmosphere by dry deposition processes, removed by wet deposition processes, or were advected out of the Four Corners States. It was assumed that 2% on a molar basis of the SO_x emissions were in the form of primary SO_4. Of the SO_x emitted in the study region, a little over 60% was estimated to be removed by dry deposition processes, nearly 15% removed by precipitation scavenging, nearly 10% advected out of the Four Corners States, and nearly 15% transformed to SO_4. SO_2 is a reactive gas, which is believed to be more effectively removed from the atmosphere by dry deposition processes than are fine particulates such as SO_4 and FPM. The regional budget % estimates in Table 4 varied little by scenario year.

4. SUMMARY

A two-dimensional Eulerian air pollutant transport model was used in an air quality study of the Four Corners region conducted for the National Commission on Air Quality. The regional modeling methodology and some sample results from the regional air quality analysis are presented in this paper. One major advantage of the regional transport model that was employed is that its solution involves the calculation of transfer coefficients that relate emissions to ambient concentrations and deposition and which can be used repeatedly to evaluate alternative scenarios and regulatory policies which represent different emission source configurations. The regional transport model was used in the calculation of the concentration and deposition of SO_2, SO_4 and FPM and these estimates were used as inputs to regional atmospheric visibility and mass budget calculations. Previous studies have shown that the methods used in the regional air quality analysis give good agreement when comparing observed and estimated values (Nochumson 1978, Nochumson et al. 1979, Nochumson 1981).

5. SYMBOLS

E_{ki} = the emission rate for species k in cell i.

c_{ki} = the concentration of species k in cell i.

c_{kij} = the concentration of species k at the interface between cells i and j.

c_{kbi} = the concentration of species k at the boundary of cell i. It is zero for interior cells.

a_{kij} = a weighting factor that relates the concentrations in two adjacent cells to the concentrations at the cell face when advective flow is from cell i to cell j.

a_{kbi} = analogous to a_{kij} but it applies when a cell is at the boundary of the system of grid cells.

U_{ij} = the volumetric air flow rate from cell i to cell j.

U_{bi} = the volumetric air flow rate across the boundary of cell i. It is zero for interior cells.

w_{ij} = the length of the cell face between cells i and j.

H = the depth of the mixing layer.

w_{ij} = the length of the cell face between the boundary and cell i.

u_{ij} = the average wind speed through the mixing depth when the direction of the wind component perpendicular to the cell face is from cell/i to cell j.

u_{bi} = the average wind speed through the mixing depth when the direction of the component perpendicular to the cell face is from the boundary to cell i. It is zero for interior cells.

A_i = the ground area of cell i.

V_i = the volume of cell i.

k_{ti} = the first order transformation rate parameter for cell i.

k_{rki} = the first order removal rate parameter for species k in cell i.

V_{dki} = the dry deposition velocity for species k in cell i.

TABLE 4

REGIONAL BUDGETS FOR SULFUR OXIDES AND PRIMARY FINE PARTICULATES

		Scenario Year							
		1980 Baseline		1987 Mid		1995 Mid		1995 High	
Species	Process	g/s	%	g/s	%	g/s	%	g/s	%
Primary Fine Particulates	Emission	363	100.0	650	100.0	922	100.0	1 376	100.0
	Deposition								
	Dry	118	32.4	198	30.5	275	29.8	394	28.7
	Wet	137	37.7	232	35.7	322	35.0	462	33.6
	Advective								
	Transport	109	34.3	220	33.8	324	35.2	519	37.7
Sulfur Dioxide[a]	Emission	1 867	98.0	2 555	98.0	3 415	98.0	4 173	98.0
	Deposition								
	Dry	1 206	63.3	1 630	62.5	2 166	62.1	2 649	62.2
	Wet	271	14.2	371	14.2	496	14.2	608	14.3
	Advective								
	Transport	151	7.9	234	9.0	315	9.0	402	9.4
Particulate Sulfate[a]	Emission	38	2.0	52	2.0	70	2.0	85	2.0
	Deposition								
	Dry	83	4.3	110	4.2	145	4.2	173	4.1
	Wet	96	5.1	129	5.0	171	4.9	204	4.8
	Advective								
	Transport	98	5.1	134	5.1	193	5.6	222	5.2

[a]Expressed as g/s of sulfur.

k_{waji} = the first order wet deposition rate parameter of species k in cell i.

P_i = the precipitation rate in cell i.

σ = the ratio of the molecular weight of the secondary pollutant, M_2, to the molecular weight of the primary pollutant, M_1.

6. ACKNOWLEDGMENTS

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